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Effect of material variation on the biomechanical behaviour of orthodontic fixed appliances: a finite element analysis

Papageorgiou, Spyridon N ; Keilig, Ludger ; Hasan, Istabrak ; Jäger, Andreas ; Bourauel, Christoph

Abstract: INTRODUCTION Biomechanical analysis of orthodontic tooth movement is complex, as many different tissues and appliance components are involved. The aim of this finite element study was to assess the relative effect of material alteration of the various components of the orthodontic appliance on the biomechanical behaviour of tooth movement. METHODS A three-dimensional finite element solid model was constructed. The model consisted of a canine, a first, and a second premolar, including the surrounding tooth-supporting structures and fixed appliances. The materials of the orthodontic appliances were alternated between: (1) composite resin or resin-modified glass ionomer cement for the adhesive, (2) steel, titanium, ceramic, or plastic for the bracket, and (3) -titanium or steel for the wire. After vertical activation of the first premolar by 0.5mm in occlusal direction, stress and strain calculations were performed at the periodontal ligament and the orthodontic appliance. RESULTS The finite element analysis indicated that strains developed at the periodontal ligament were mainly influenced by the orthodontic wire (up to +63 per cent), followed by the bracket (up to +44 per cent) and the adhesive (up to +4 per cent). As far as developed stresses at the orthodontic appliance are concerned, wire material had the greatest influence (up to +155 per cent), followed by bracket material (up to +148 per cent) and adhesive material (up to +8 per cent). LIMITATIONS The results of this in silico study need to be validated by in vivo studies before they can be extrapolated to clinical practice. CONCLUSION According to the results of this finite element study, all components of the orthodontic fixed appliance, including wire, bracket, and adhesive, seem to influence, to some extent, the biomechanics of tooth movement.

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TITLE PAGE

Effect of material variation on the biomechanical behavior of orthodontic fixed appliances: a finite element analysis

Spyridon N. Papageorgiou,[1,2], Ludger Keilig,[2,3], Istabrak Hasan,[2,3], Andreas Jäger,[1], and Christoph Bourauel,[2]

[1]Department of Orthodontics, School of Dentistry, University of Bonn, Bonn, Germany.

[2]Department of Oral Technology, School of Dentistry, University of Bonn, Bonn, Germany.

[3]Department of Prosthodontics, Preclinical Education and Dental Materials Science, School of Dentistry, University of Bonn, Bonn, Germany.

Running title: Variation of material properties of orthodontic fixed appliances

Corresponding author:

Prof. Christoph Bourauel, Department of Oral Technology, University of Bonn, Welschnonnenstr. 17, 53111, Bonn, Germany, Tel.: +49-(0)228-287-22332, Fax: +49-(0)228-287-22385, E-mail: bourauel@uni-bonn.de.

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ABSTRACT

Introduction: Biomechanical analysis of orthodontic tooth movement is complex, as many different tissues and appliance components are involved. The aim of this finite element study was to assess the relative effect of material alteration of the various components of the orthodontic appliance on the biomechanical behavior of tooth movement.

Methods: A three-dimensional FE solid model was constructed. The model consisted of a canine, a first, and a second premolar, including the surrounding tooth-supporting structures and fixed appliances. The materials of the orthodontic appliances were alternated between: (a) composite resin or resin-modified glass-ionomer cement for the adhesive, (b) steel, titanium, ceramic or plastic for the bracket, and (c) β-titanium or steel for the wire. After vertical activation of the first premolar by 0.5 mm in occlusal direction, stress and strain calculations were performed at the periodontal ligament and the orthodontic appliance.

Results: The finite element analysis indicated that strains developed at the periodontal ligament were mainly influenced by the orthodontic wire (up to +63%), followed by the bracket (up to +44%) and the adhesive (up to +4%). The developed stresses at the orthodontic appliance, wire material had the greatest influence (up to +155%), followed by bracket material (up to +148%) and adhesive material (up to +8%).

Conclusion: According to the results of this finite element study, all three components of the orthodontic fixed appliance (wire, bracket, and adhesive) seem to influence, to some extent, the biomechanics of tooth movement.

Keywords: orthodontics; tooth movement; material properties; stress; strain; finite element

MAIN TEXT

Introduction

Orthodontic tooth movement is based on the ability of surrounding bone and periodontal ligament (PDL) to react to a mechanical stimulus with remodeling processes. Application of an orthodontic force system to a tooth causes displacement, stresses and strains in the structures involved [Melsen, 1980; Davidovitch et al., 1980], while mechanotransductory processes are translated to cell-to-cell signaling [Turner and Pavalko, 1998]. There has been evidence of a direct or indirect correlation of the calculated stress/strain values in the PDL with the distributions of osteoclasts in the alveolar bone and PDL of rats or monkeys [Melsen, 2001; Kawarizadeh et al., 2004; Cossetin et al., 2012]. Thus, tensions developed in the ligament and alveolar bone provide indications of a favorable or unfavorable tooth movement [Tom and Eberhardt, 2003]. The magnitude of generated tension varies inversely with the area in which the load is applied [Khouw and Goldhaber, 1970; Quinn and Yoshikawa, 1985] and with the type of accompanying remodeling.

In recent years, the increased esthetic demands of patients who seek orthodontic treatment have led to the development of various esthetic materials, including orthodontic brackets. The two primary types of esthetic brackets are the ceramic and the plastic brackets [Russell, 2005; Gkantidis et al., 2012]. Unlike metallic brackets, ceramic brackets have high brittleness and increased susceptibility to fracture and thus are more prone to complications for the orthodontist [Birnie, 1990; Karamouzos et al., 1997], while also causing more damage to the enamel during debonding than metallic brackets [Eliades et al., 1993]. The main disadvantages of plastic brackets on the other side are reduced torque transmission, color changes, morphological disturbances, and structural or hardness derangements [Alkire et al., 1997; Eliades et al., 2004; Gioka and Eliades, 2004]. Moreover, the clinical efficiency of ceramic and plastic brackets might be considerably reduced during treatment due to intraoral aging [Eliades and Bourauel, 2005; Gkantidis et al., 2012]. The biomechanical behavior of the bracket is important to the orthodontist, as the risk of bracket wing fracture is increased with esthetic brackets [Karamouzos et al., 1997; Scott, 1988], which leads to increased chair time, patient discomfort and potential aspiration of the wing fragment. This is attributed to the almost non-existing plastic deformation of ceramic brackets and their significantly lower fracture strength compared to metallic brackets. Additionally, the developed stresses in the bracket and its distribution to the underlying adhesive-bracket interface might lead to crack initiation and propagation and subsequent debonding of the bracket [Higg et al., 2010]. The elastic properties of the bracket and the adhesive have been associated with differences in the corresponding bond strength [Haydar et al., 1999]. Finally, development of excessive stresses in the wire might lead to permanent deformation, which can hamper tooth movement.

The relative influence on the various materials of orthodontic appliances on the resulting tooth movement has not been adequately studied. Two recent systematic reviews of clinical trials in humans indicated that there is limited evidence regarding both bracket material and wire material [Papageorgiou et al., 2014a; Papageorgiou et al., 2014b]. This lies in part in the complexity of the biomechanical behavior of the complex between dental tissues and the orthodontic fixed-appliances, as many tissues or materials with different properties are involved, including bone, PDL, tooth structures, adhesive, bracket and wire.

The Finite Element (FE) method has been suggested as a solution for complex biomechanical questions and has been applied in several cases in orthodontics [Cattaneo et al., 2005; Bourauel et al., 2007] in order to assess the center of resistance [Reimann et al., 2007; Kettenbeil et al., 2013; Viecilli et al., 2013], various biomechanical aspects of tooth movement [Tominaga et al., 2012; Tominaga et al., 2014], different bracket [Huang et al., 2009; Huang et al., 2012], anchorage [Reimann et al., 2009; Stahl et al., 2009; Chatzigianni et al., 2011; Largura et al., 2014] or surgical [MacGinnis et al., 2014; Kim et al., 2014] treatment modalities, debonding [Algera et al., 2011; Holberg et al., 2014; Milheiro et al., 2014] and retention procedures [Jahanbin et al., 2014]. The reliability of FE analyses is dependent not only on the loading configuration, but also on the geometry of the structure and the material properties [Huiskes and Chao, 1983; Cattaneo et al., 2005]. Experimental validation studies of the FE analyses [Algera et al., 2011] are also encouraged, whenever possible.

The primary objective of the present *in silico* study was to assess the influence of material variations on the strains induced at the PDL. The secondary objective was to assess the effect of material variation on the stresses developed at the orthodontic bracket.

Materials and methods

A three-dimensional (3D) solid model was constructed including a lower right canine, first premolar and second premolar, with the corresponding PDLs and alveoli. All separate PDLs had uniform thickness of 0.2 mm and all separate alveoli had a uniform thickness of 0.5 mm. A partial orthodontic fixed appliance was constructed with adhesive layers (mean thickness 0.2 mm) and brackets on each of the three teeth, while a round 0.41 mm (0.016 inch) wire was inserted in all brackets slots and ligated with two ligatures. For all teeth the same bracket was used, based on CAD/CAM data from the discovery® (Dentaurum, Ispringen, Germany) brackets, provided by the manufacturer, with a slot size of 0.46 x 0.64 mm (0.018 x 0.025 inch) and placed in the middle of the buccal side of the clinical crown (Figure 1).

Based on these 3D solid models, an FE mesh was created to make a node-to-node connection between bracket, adhesive, tooth, PDL, and alveolar bone. An FE mesh of the wire was created separately from the bracket to allow the wire to slide through the bracket slots. A free mobility of the wire within the bracket slot was given by performing contact analyses based on the Coulomb friction model in the FE program used (MSC.Marc/Mentat v. 2010, MSC Software Corp., Santa Ana, CA, USA). This means that the wire is not deformed until it comes into contact with the slot walls and thus the wire mobility was restricted by the slot walls and the ligature, respectively. A frictional coefficient between the bracket and the wire of 0.1 was used. The 3D FE model consisted of 624,118 isoparametric tetrahedral solid elements (4-noded) and 756,067 nodes (Figures 1-3).

The material properties used in this study were based on previous published studies (Table 1). All materials were considered to be homogenous and isotropic apart from the PDL, which was modeled as bilinear elastic [Kettenbeil et al., 2013]. According to the objectives of this study, the following material parameters were used for the adhesive layer, the bracket and the wire in order to assess the effect of this variation on the developed stresses and strains: (I) adhesive: composite resin or Resin-Modified Glass Ionomer cement (RMGI), (II) bracket: stainless steel, titanium alloy, ceramic or plastic (polycarbonate), and (III) wire: stainless steel or β-Titanium Alloy (β-Ti). A total of 11 different models were generated with random variation of these materials.

The simulation was designed to reflect the clinical situation of a deformed wire acting on a slightly extruded first premolar. By a preliminary FE simulation, the wire was inserted in the aligned slots of the three brackets and passively secured with the ligatures. In order to simulate the activated wire, the alveolus of the first premolar was deflected by 0.5 mm in occlusal direction perpendicular to the tooth axis, while the other two alveoli were held and the ligatures were activated. The induced total equivalent strains in the PDL and the induced stresses (Von Mises stresses) in the bracket and wire of the first premolar were measured at the end of the 0.5 mm deflection phase. Mean stresses/strains across models according to the various material parameters were calculated and analyzed descriptively. All simulations of tooth movement were performed with the above-mentioned FE software. Models were created on a Dell Precision T5500 workstation (Dell, Frankfurt, Germany) and transferred to a 30-processor Dell server cluster at the Department of Oral Technology to be solved, which took an average 38-109 hours per individual simulation.

Results

The raw data of the 11 simulated models finally included are reported in the Appendix and summarized as means across models in Tables 2-4. Characteristic examples of the developed strains in the PDL, the developed stresses in the bracket and the developed stresses in the wire are illustrated in Figures 4-6, respectively.

The differences of the calculated strains at the PDL level are shown in Table 2. As can be seen, the greatest influence on strains was found, as expected, for the wire material with a mean variation of 63%. Variation of the bracket material on the other hand led to variations up to 44% according to the material. Finally, variation of the adhesive material had a minimal effect on the developed strain (4%).

The changes in the calculated stresses at the bracket level are shown in Table 3. The same tendency was shown, with the wire material exerting the highest influence (up to 152%), followed by the bracket material (up to 148%) and by the adhesive material (up to 8%). The same observation was made for the stresses at the wire level, where the wire material exerted the highest influence (up to 155%), followed by the bracket material (up to 126%) and by the adhesive material (up to 7%).

Discussion

In this study the relative contribution of the adhesive's, bracket's or wire's materials to the developed stresses and strains was investigated *in silico*. It was observed that the strains induced at the PDL level were affected mainly by the wire, followed by the bracket and finally, minimally, by the used adhesive. The same observation was made for the developed stresses at the bracket or the wire level.

The finite element method enables us to answer complex biomechanical questions in the field of orthodontics via simulation; moreover, it enables investigators to predict the behavior of biological structures in many specific situations. However, any solutions obtained via FEM simulation will be numerical approximations. Although many measurements cannot be taken *in vivo*, they can nevertheless contribute useful information to clinical investigations.

The variation of the used materials had a profound effect on the developed strains in the PDL. This effect was more profound for the bracket's and wire's material, but was also marginally existent for the adhesive's material. It is therefore important to take this factor into account when making clinical decisions in orthodontics, as the developed strains in the PDL are directly associated with the biological processes of tooth movement [Melsen, 2001; Kawarizadeh et al., 2004; Cossetin et al., 2012]. There is some evidence that, unlike light forces, heavy forces might cause necrosis (hyalinization) of the PDL, undermining bone resorption, and play a role in root resorption [Reitan, 1957; Krishnan and Davidovitch, 2006].

Material variations of the adhesive, bracket or wire influenced the developed stresses at the fixed appliance (bracket and wire), with the effect being stronger for the last two. This might have an influence on the breakage rate of the bracket wings or on the bond failure between bracket and adhesive. Comparing this study with similar works is limited, due to absence of the latter. The influence of changes in the adhesive's Young's modulus on the developed stresses in the bracket was likewise found to be minimal in a previous study [Knox et al., 2001AJO]. In another simplified FE study, the effect of bracket material variation on the resulting stresses in the bracket was found to be limited [Ranjit and Kim, 2014]. However, modeling and activation conditions differed from the present study and no direct comparison is possible. Finally, the stresses developed at the wire, were influenced by the material variation of both the wire and the bracket as well. This should also be taken into account, for choosing the material of the fixed appliance, as the excessive stresses developed in the wire might lead to its permanent plastic deformation.

There are additional factors that might influence the biomechanical behavior of the fixed appliance. Ghosh et al. [1995] investigated various designs of ceramic brackets and reported significant variation in the stresses in the bracket according to the bracket design, with uneven stress distributions with increased stresses at the edges of brackets with sharp lines and angles. Moreover, significant differences in the tie-wing tensile fracture strength of semi-twin and true-twin brackets have been reported [Johnson et al., 2004]. The former perform better, as the bulk piece of ceramic that connect the mesial and the distal wings has a cross-stabilizing effect. Additionally, Gkantidis et al. [2012] reported that ceramic brackets present irregularities in the inner slot surface, which increase pressure expressed by the wire and lead to attrition, something that was not modeled in the present study. Likewise, all brackets modeled consisted from a single material phase and no different materials were used for the tie-wings and base of the bracket, as is sometimes done for metallic brackets [Zinelis et al., 2005].

The strengths of this study include the bilinear modeling of the PDL, which is more accurate than the usually-used simplified linear modeling of the PDL [Ziegler et al., 2005; Dong-Xu et al., 2011]. All material properties used were based on previous studies. To reduce the systematic error, no absolute values were considered to draw the conclusion, only the differences between the simulations. Since all simulations were affected by the simplification effects to the same extent, the analysis of the differences resulted in an additional increase of validity.

The limitations of this study include the existing play between the bracket and wire of the simulated model, which could influence the results [Tominaga et al., 2012]. However, this was the same for all tested models. On the other hand a heavier or a rectangular wire would not make sense, as the stainless steel was amongst the tested wire materials and stainless steel rectangular wires are not used for initial alignment. To reduce the number of equations to be solved, the teeth were not differentiated into enamel, dentine, pulp, and cementum but were provided uniformly with the elasticity parameters of dentine. In view of the minor forces applied, the influence of this simplification is negligible because no substantial deformation of the dental hard tissue was to be expected. For the same reason, the bone was not differentiated into cancellous and cortical bone [Bourauel et al., 1999; Vollmer et al., 2000]. Finally, superelastic nickel-titanium wires could not be modeled for this experiment, despite their wide clinical usefulness [Pandis and Bourauel, 2010], as they caused computational problems, due to the heavy data load.

Conclusions

According to this *in silico* study, the following conclusions can be drawn:

- The magnitude of the strains in the PDL was found to be dependent on the wire, bracket and adhesive material. The largest influence was noted for the wire material, followed by the bracket material.
- Likewise, the wire, bracket and adhesive materials had a direct influence on the severity of stresses developed at the bracket. Again, the largest influence was noted for the wire material, followed by the bracket and the adhesive materials.

As a result, the biomechanical behavior of the orthodontic appliances should also be taken into account in clinical decision making together with esthetic reasons and patient preferences. However, clinical studies need to be performed to verify these findings.

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Conflict of interest

No existing conflicts of interest. Mr. Papageorgiou is receiving funds by the Clinical Research Unit 208 (University of Bonn, Bonn, Germany).

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TABLES

Table 1. Material properties used in this study.

Material	Young's modulus (MPa)	Poisson's ratio
Bone [Tominaga et al., 2014]	2,000	0.30
Periodontal ligament [Kettenbeil et al., 2013]	bilinear: 0.05/0.20 ultimate strain ε_{12}: 7.0%	0.30
Tooth [Tominaga et al., 2014]	20,000	0.30
Adhesive – composite resin [Lin et al., 2011]	8,823	0.25
Adhesive – RMGI [Hioki et al., 2007]	7,600	0.30
Bracket – stainless steel [Huang et al., 2009]	200,000	0.30
Bracket – titanium [Lacoursière, 2010]	114,000	0.30
Bracket – ceramic [Ranjit and Kim, 2014]	379,000	0.29
Bracket – plastic [Gkantidis et al., 2012]	2,200	0.30
Wire – stainless steel [Huang et al., 2009]	200,000	0.30
Wire – β-Ti [Brantley and Eliades, 2001]	65,000	0.30

RMGI, resin-modified glass ionomer cement; β-Ti, β-Titanium alloy

Table 2. Obtained strains in the PDL according to the various material properties.

Factor	Material	Mean strain	Strain change	Strain change %
Adhesive material	Composite resin	0.164	*Ref*	*Ref*
	RMGI	0.170	+0.006	+4%
Bracket material	Ceramic	0.133	*Ref*	*Ref*
	Stainless steel	0.178	+0.045	+34%
	Titanium	0.191	+0.058	+44%
	Plastic	0.191	+0.058	+44%
Wire material	β-Ti	0.136	*Ref*	*Ref*
	Stainless steel	0.221	+0.085	+63%

Ref, reference; RMGI, resin-modified glass ionomer cement; β-Ti, β-Titanium alloy

Table 3. Obtained stresses (MPa) in the bracket and wire according to the various material properties.

Factor	Material	Bracket		
		Mean stress	Stress change	Stress change %
Adhesive material	Composite resin	27.3	*Ref*	*Ref*
	RMGI	29.4	+2.1	+8%
Bracket material	Ceramic	14.7	*Ref*	*Ref*
	Plastic	25.0	+10.3	+70%
	Stainless steel	30.6	+15.9	+108%
	Titanium	36.5	+21.8	+148%
Wire material	β-Ti	18.2	*Ref*	*Ref*
	Stainless steel	45.9	+27.7	+152%

Ref, reference; RMGI, resin-modified glass ionomer cement; β-Ti, β-Titanium alloy

Table 4. Obtained stresses (MPa) in the wire according to the various material properties.

Factor	Material	Wire		
		Mean stress	Stress change	Stress change %
Adhesive material	Composite resin	101.3	*Ref*	*Ref*
	RMGI	108.1	+6.7	+7%
Bracket material	Titanium	60.8	*Ref*	*Ref*
	Stainless steel	69.0	+8.2	+14%
	Ceramic	119.3	+58.5	+96%
	Plastic	137.3	+76.5	+126%
Wire material	β-Ti	66.8	*Ref*	*Ref*
	Stainless steel	170.1	+103.3	+155%

Ref, reference; RMGI, resin-modified glass ionomer cement; β-Ti, β-Titanium alloy

FIGURE LEGENDS

Figure 1. The constructed model with its components.

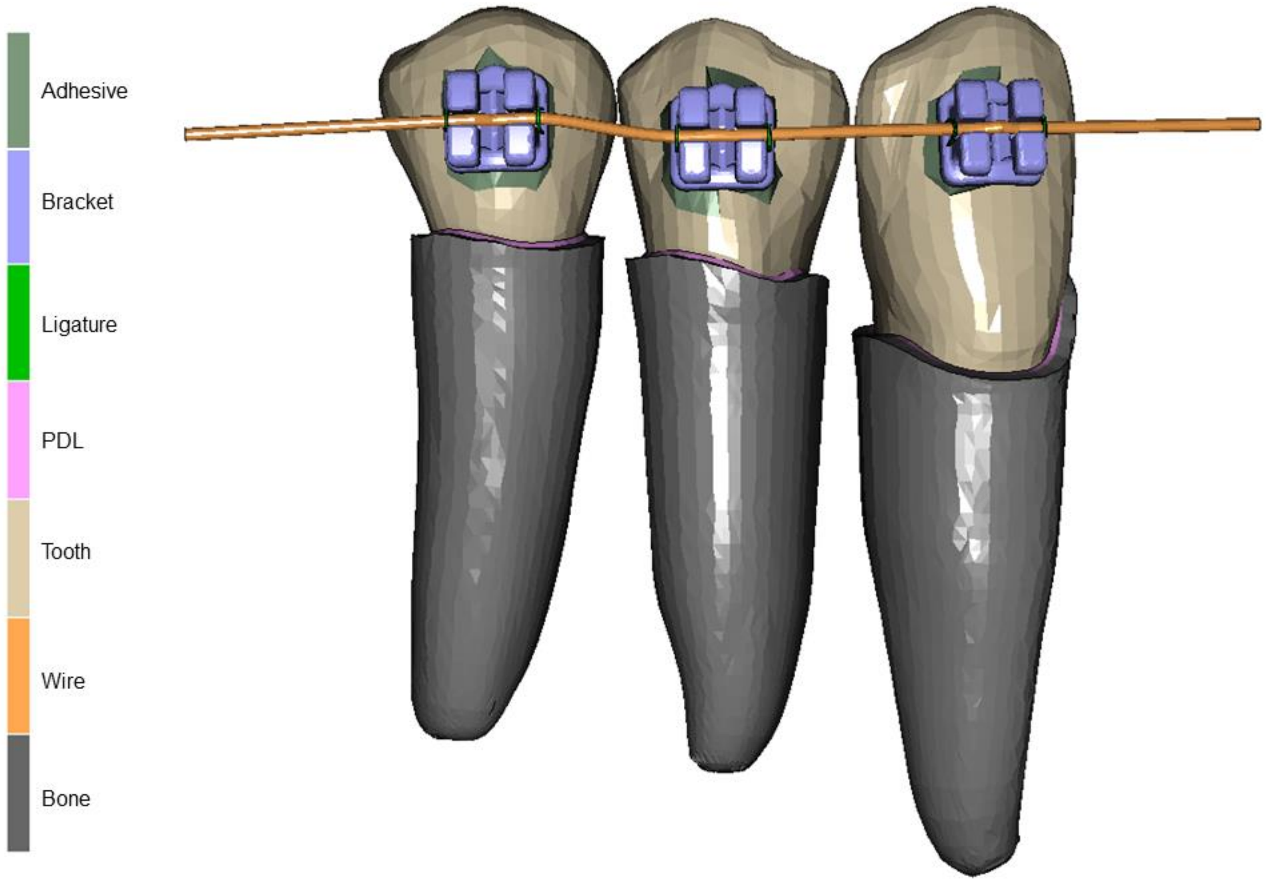

Figure 2. Details of each tooth modeled together with the components of the fixed appliance.

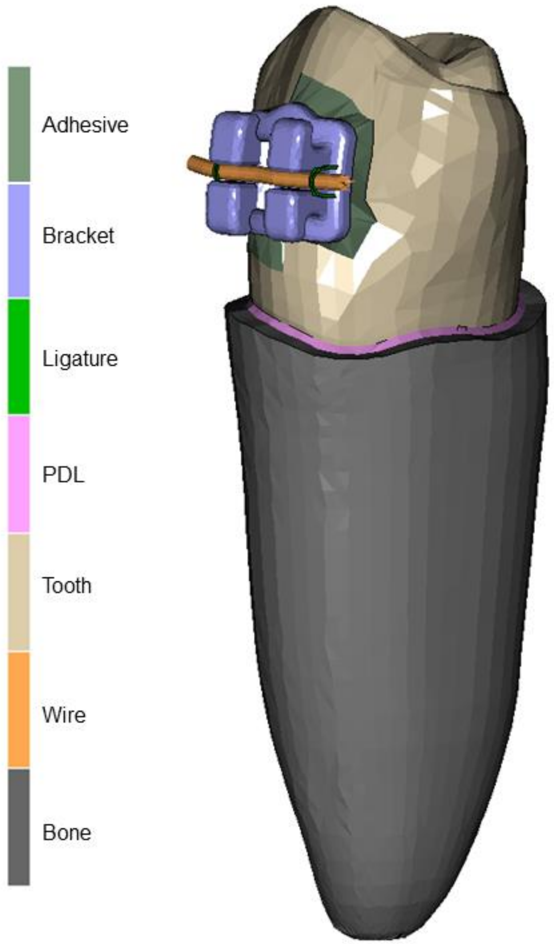

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Figure 3. Details of the modeled bracket, wire and ligatures.

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Figure 4. Example showing the distribution of total equivalent strains in the PDL.

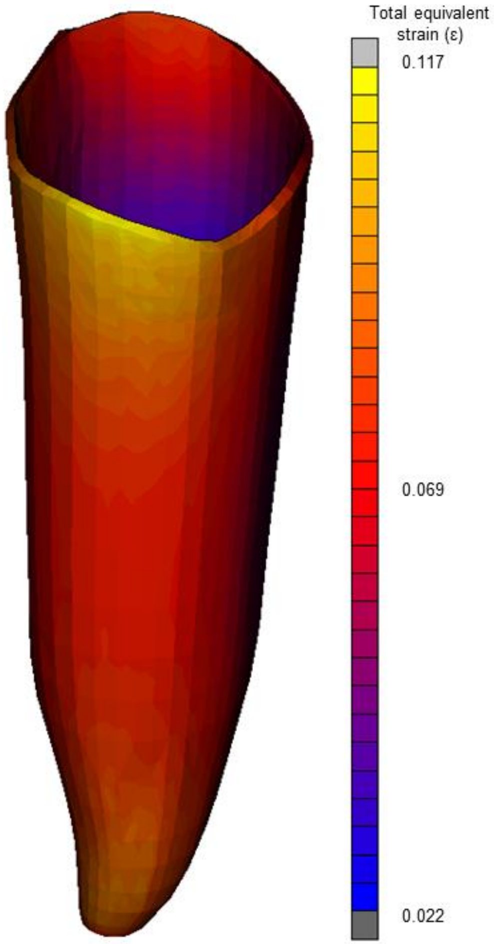


Figure 5. Example showing the distribution of von Mises stresses in the bracket.

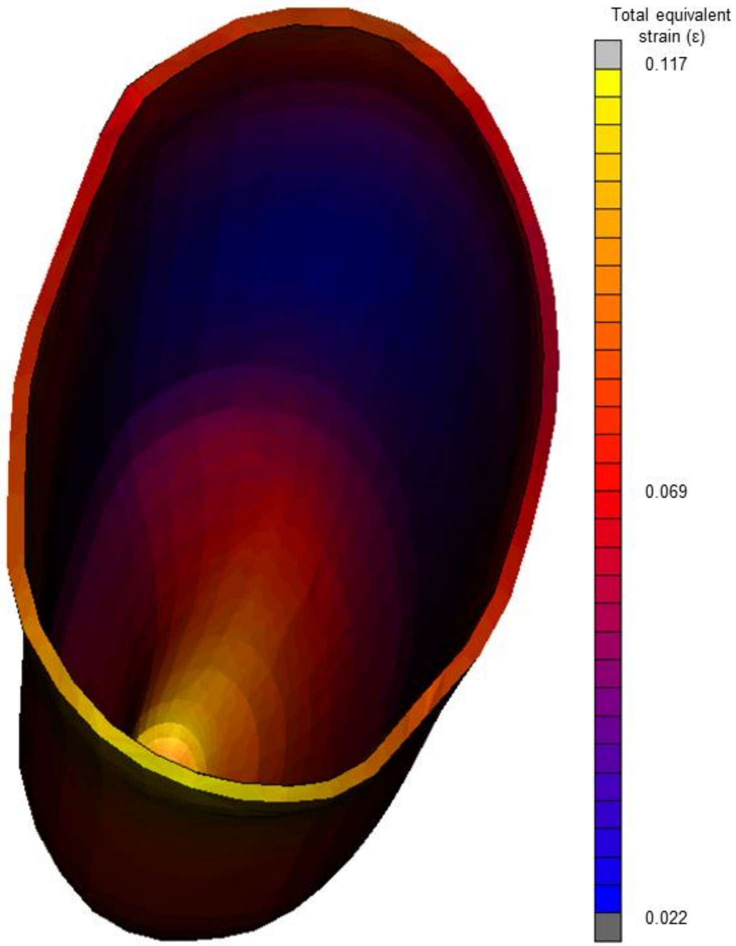
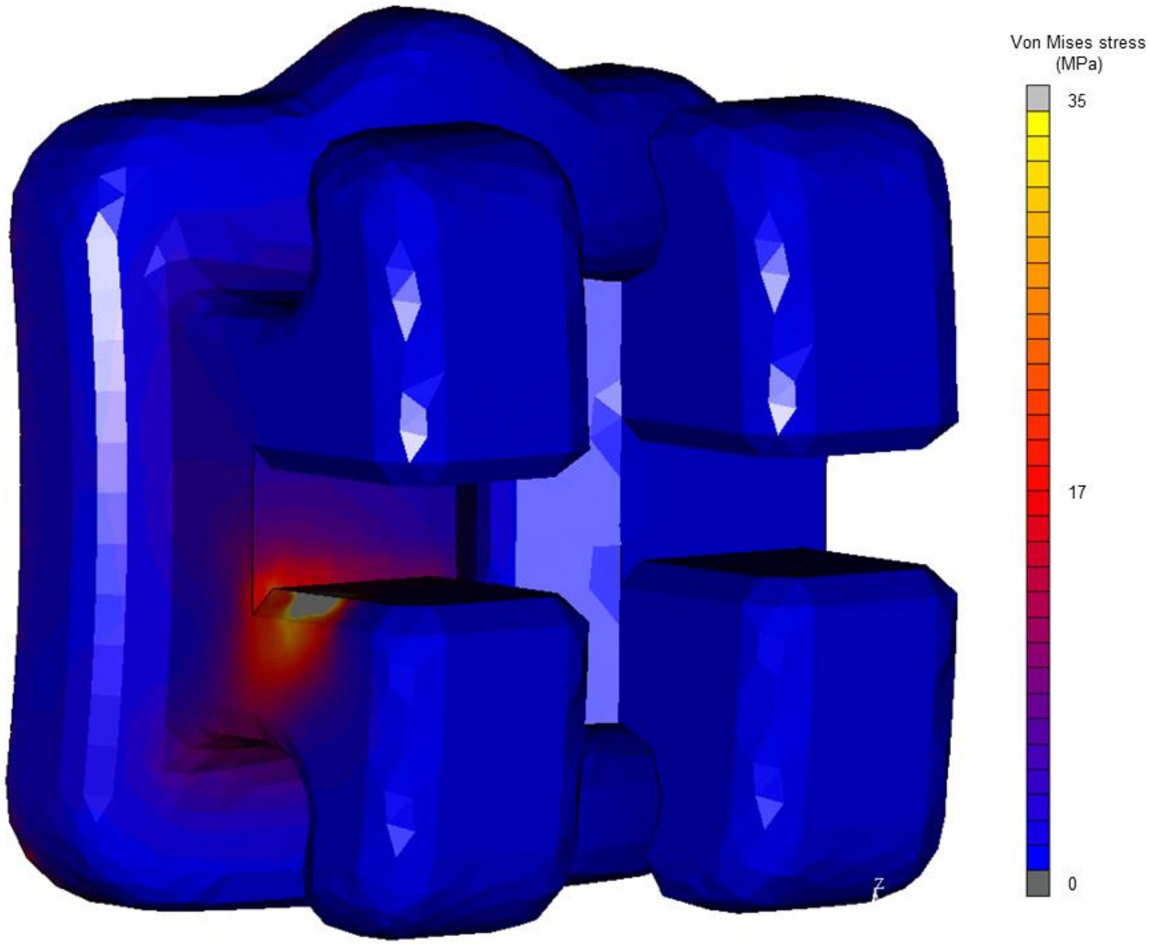


Figure 6. Example showing the distribution of von Mises stresses in the wire.



Appendix. Raw data of the 11 simulated models.

Model	Adhesive	Bracket	Wire	Strain at PDL (ε)	Von Mises stress in bracket (MPa)	Von Mises stress in wire (MPa)
A	Composite resin	Ceramic	β-Ti	0.1330	13.2204	68.9618
B	Composite resin	Plastic	β-Ti	0.1409	24.9812	60.8507
C	Composite resin	Stainless steel	Stainless steel	0.2209	46.8287	169.7300
D	Composite resin	Stainless steel	β-Ti	0.1347	16.0491	69.1556
E	Composite resin	Titanium	Stainless steel	0.2209	47.6856	169.1428
F	Composite resin	Titanium	β-Ti	0.1316	15.2447	70.1490
G	Resin-modified glass ionomer	Ceramic	β-Ti	0.1330	16.1649	68.9590
H	Resin-modified glass ionomer	Plastic	β-Ti	0.1409	24.9547	60.6569
I	Resin-modified glass ionomer	Stainless steel	Stainless steel	0.2201	42.6689	169.0624
J	Resin-modified glass ionomer	Stainless steel	β-Ti	0.1347	16.7997	69.1526
K	Resin-modified glass ionomer	Titanium	Stainless steel	0.2201	46.5052	172.5225

PDL, periodontal ligament; β-Ti, β-Titanium alloy

Supplementary material

Supplementary table. Raw data of the 11 simulated models. PDL, periodontal ligament; β-Ti, β-Titanium alloy

Model	Adhesive	Bracket	Wire	Strain at PDL (ε)	Von Mises stress in bracket (MPa)	Von Mises stress in wire (MPa)
A	Composite resin	Ceramic	β-Ti	0.1330	13.2204	68.9618
B	Composite resin	Plastic	β-Ti	0.1409	24.9812	60.8507
C	Composite resin	Stainless steel	Stainless steel	0.2209	46.8287	169.7300
D	Composite resin	Stainless steel	β-Ti	0.1347	16.0491	69.1556
E	Composite resin	Titanium	Stainless steel	0.2209	47.6856	169.1428
F	Composite resin	Titanium	β-Ti	0.1316	15.2447	70.1490
G	Resin-modified glass ionomer	Ceramic	β-Ti	0.1330	16.1649	68.9590
H	Resin-modified glass ionomer	Plastic	β-Ti	0.1409	24.9547	60.6569
I	Resin-modified glass ionomer	Stainless steel	Stainless steel	0.2201	42.6689	169.0624
J	Resin-modified glass ionomer	Stainless steel	β-Ti	0.1347	16.7997	69.1526
K	Resin-modified glass ionomer	Titanium	Stainless steel	0.2201	46.5052	172.5225